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# Improvement of Numerical Integration Formulas by Iterated Cubic Splines

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### Abstract

We improve numerical integration with a fixed number of evaluation points based on iterated cubic splines. Some numerical examples are given to illustrate usefulness of our methods.

## 1. Introduction and Description of Methods

Iterated cubic splines are useful for order-preserving approximation to a given function. There is computational evidence that they give better results than a single spline ([1], [3]). Recently we have considered an application of the iterated cubic splines to evaluation of integrals on subintervals $[x_j, x_{j+1}]$ or the ratios to the whole interval [0, 1] required in statistics:

$$\text{(1)} \qquad \int_{x_j}^{x_{j+1}} f(x)\,dx \quad \text{or} \quad \int_{x_j}^{x_{j+1}} f(x)\,dx \Big/ \int_0^1 f(x)\,dx \quad \text{for some or all } j \quad (0 \leq j \leq n-1)$$

where let $n \geq 1$, $x_j = jh$ $(= j/n)$ ([5]). Use the notation: $f_j = f(x_j)$, $s_{m,j} = s_m(x_j)$, $s'_{m,j} = s'_m(x_j)$ and $f_{j+1/2} = f((x_j + x_{j+1})/2)$. Then, the iterated cubic splines $s_m$ $(m \geq 0)$ are recursively defined as follows. First, let $s_0$ be the usual cubic spline interpolant of $f$ on the uniform partition of [0, 1] with knots $x_j$, i.e.,

$$\text{(2)} \qquad s_{0,j} = f_j \quad (0 \leq j \leq n) \quad \text{subject to} \quad \Delta^k s'_{0,0} = \nabla^k s'_{0,n} = 0$$

where from now on, $k \in \{0, 1, \ldots, n-1\}$ is fixed and $\Delta$ $(\nabla)$ is the forward (backward) difference operator. Next, let $s_m$ $(m \geq 1)$ be the cubic spline interpolant of $s'_{m-1}$ on the same uniform partition, i.e.,

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(3) $$s_{m,j}=s'_{m-1,j}\quad(0\leq j\leq n)\ \text{ subject to }\ \Delta^k s'_{m,0}=\nabla^k s'_{m,n}=0.$$

In computation of the iterated cubic splines $s_m$ $(m\geq 0)$, it is convenient to rewrite the end condition $\Delta^k s'_{m,0}=0$ as follows:

(4) $$c_k s'_{m,0}+s'_{m,1}=L_k(d_1, d_2, \ldots, d_{k-1})$$

where for $c_k$, $L_k$ and computational comment, see [3] or [5]. The end condition $\Delta^9 s'_{m,0}=0$ used in the numerical examples is equivalent to

(5) $$(71/265)s'_{m,0}+s'_{m,1}=(92017d_1-24637d_2+6567d_3-1715d_4+419d_5-87d_6+13d_7-d_8)/57240$$

where $d_j$ is the right hand side of the consistency relation for the cubic spline:

(6) $$(s'_{m,j+1}+4s'_{m,j}+s'_{m,j-1})/6=(s_{m,j+1}-s_{m,j-1})/(2h)\quad(=d_j).$$

For a periodic function $f$, the end conditions (2)—(3) are to be replaced by

(7) $$s^{(r)}_{m,0}=s^{(r)}_{m,n}\quad(0\leq r\leq 2,\ m\geq 0).$$

The following asymptotic error estimates for the $m$-th derivative $f^{(m)}$ by the $m$-th iterated cubic spline $s_m$ are based on results in [3] (nonperiodic) and [6] (periodic) where $C^q_p[0, 1]$ denotes the set of periodic functions in $C^q(-\infty, \infty)$ with period one.

**Lemma** ([3]—[6]). *For $1\leq m\leq 9$ and $f\in C^{10}_p[0, 1]$ (periodic case) and $1\leq m\leq k\leq n-1$, $k\leq 9$ and $f\in C^{10}[0, 1]$ (nonperiodic case), then*

(8) $$s_{m,j}=f^{(m)}_j-m\left\{\frac{h^4}{180}f^{(m+4)}_j-\frac{h^6}{1512}f^{(m+6)}_j\right\}-c_m h^8 f^{(m+4)}_j+O(h^L)\quad(0\leq j\leq n)$$

*where $c_1=1/25920$, $L=10-m$ or $L=k+1-m$ for periodic case or nonperiodic case. Note that the $h^8$ term is absorbed into the order term for $m\geq 2$.*

By making use of the iterated cubic splines $s_m$ as apporximation to the derivatives in the asymptotic error estimate in Simpson's rule:

(9) $$\int_{x_j}^{x_{j+1}} f(x)\,dx-(h/6)(f_j+4f_{j+1/2}+f_{j+1})=\sum_{k=1}^{3}(-1)^k h^{2k+2} C_k\,\Delta f^{(2k+1)}_j+O(h^{11}),$$

we can get an improvement of the rule based on the iterated splines:

$$(10) \qquad S_{m,j}(h)=(h/6)(f_j+4f_{j+1/2}+f_{j+1})+\sum_{k=1}^{m}(-1)^k h^{2k+2}\overline{C}_k \Delta s_{2k+1,j} \quad (0\leq m\leq 3)$$

where $(C_1, C_2, C_3)=(1/2880, 1/96768, 1/3686400)$ and $(\overline{C}_1, \overline{C}_2, \overline{C}_3)=(1/2880, 1/96768, 67/1059200)$. For the errors in $S_{m,j}(h)$, we obtain

**Theorem 1.** *Let* $k\in\{2m+3, 2m+4, \ldots, n-1\}$ *and* $k\leq 9$ *be fixed.* (*This restriction on* $k$, *defined in* (2) *and* (3), *is necessary in the nonperiodic case only.*) *If* $f\in C_p^{10}[0, 1]$ *or* $\in C^{10}[0, 1]$, *then*

$$\int_{x_j}^{x_{j+1}} f(x)\,dx-S_{m,j}(h)=O(h^{2m+5}) \quad (0\leq m\leq 3).$$

Similarly as in Simpson's rule, the asymptotic relation is known for the midpoint one:

$$(11) \qquad \int_{x_j}^{x_{j+1}} f(x)\,dx-h/f_{j+1/2}=\sum_{k=1}^{3}(-1)^{k+1}h^{2k}D_k\Delta f_j^{(2k-1)}+O(h^9)$$

from which we get the following formulas:

$$(12) \qquad M_{m,j}(h)=hf_{j+1/2}+\sum_{k=1}^{m}(-1)^{k+1}h^{2k}\overline{D}_k\Delta s_{2k-1,j} \quad (0\leq m\leq 3)$$

where $(D_1, D_2, D_3)=(1/24, 7/5760, 31/967680)$ and $(\overline{D}_1, \overline{D}_2, \overline{D}_3)=(1/24, 7/5760, 17/64512)$. For the errors in $M_{m,j}(h)$, we obtain

**Theorem 2.** *Let* $k\in\{2m+1, 2m+2, \ldots, n-1\}$ *and* $k\leq 7$ *be fixed.* (*This restriction on* $k$, *defined in* (2) *and* (3), *is necessary in the nonperiodic case only.*) *If* $f\in C_p^8[0, 1]$ *or* $\in C^8[0, 1]$, *then*

$$\int_{x_j}^{x_{j+1}} f(x)\,dx-M_{m,j}(h)=O(h^{2m+3}) \quad (0\leq m\leq 3).$$

*Proof.* Under the condition on $k$, $m$ and $f$ in Theorem 2, we have only to check

$$(13) \qquad s_{m,j}=f_j^{(m)}-m\left\{\frac{h^4}{180}f_j^{(m+4)}-\frac{h^6}{1512}f_j^{(m+6)}\right\}+O(h^L) \quad (0\leq j\leq n)$$

where $L=8-m$ or $L=k+1-m$ for periodic case or nonperiodic case.

We can also consider improvement of the product trapezoidal rule when $w(x)=x^{\alpha}$ $(\alpha>-1)$ or $\ln(x)$ for which the following asymptotic error formula is obtained:

$$\int_{x_j}^{x_{j+1}} w(x)f(x)\,dx-h\{p_0(j)f_j+q_0(j)f_{j+1}\}$$
$$=\sum_{m=1}^{3} h^{2m}\{p_m(j)f_j^{(2m-1)}+q_m(j)f_{j+1}^{(2m-1)}\}+O(h^{9+\min(0,\alpha)}) \text{ or } O(h^9|\ln(h)|). \tag{14}$$

Here, first coefficients $q_m$ $(=q_m(j))$ $(0\leq m\leq 3)$ are determined by substitution of $(x-x_j)^{2m}$ $(1\leq m\leq 3)$, $(x-x_j)^7$ into (14) without order terms, and next coefficients $p_m$ $(=p_m(j))$ are successively done by substituting $(x-x_j)^{2m-1}$ $(1\leq m\leq 3)$ as follows:

$$\begin{aligned}
&17hq_0=-4c_7+14c_6-35c_4+42c_2,\ 34hq_1=4c_7-14c_6+35c_4-25c_2\\
&204hq_2=-2c_7+7c_6-9c_4+4c_2,\ 12240hq_3=12c_7-25c_6+20c_4-7c_2\\
&17hp_0=4c_7-14c_6+35c_4-42c_2+17c_0,\ 34hp_1=4c_7-14c_6+35c_4-59c_2+34c_1\\
&204hp_2=-2c_7+7c_6-26c_4+34c_3-13c_2,\\
&12240hp_3=17c_7-59c_6+102c_5-65c_4+10c_2
\end{aligned} \tag{15}$$

where $c_m(=c_m(j))=\int_0^1 \theta^m w(x_j+h\theta)\,d\theta$ are successively determined as follows:

for $w(x)=x^{\alpha}$, $h(1+\alpha)c_0=x_{j+1}^{1+\alpha}-x_j^{1+\alpha}$, $h(m+1+\alpha)c_m=x_{j+1}^{1+\alpha}-mjhc_{m-1}$ $(m\geq 1)$;

for $w(x)=\ln(x)$, $hc_0=x_{j+1}\ln(x_{j+1})-x_j\ln(x_j)-h$,

$$h(m+1)c_m=x_{j+1}\ln(x_{j+1})-mjhc_{m-1}+mh/(m+1)\quad (m\geq 1).$$

For $\alpha=0$, $(p_0, p_1, p_2, p_3)=(q_0, -q_1, -q_2, -q_3)=(1/2, -1/12, 1/720, -1/30240)$, i.e., (14) reduces to a special case of the well-known Euler-Machaurin summation formula. Use $s_m$ as an approximation of $f^{(m)}$ to give the following integration formulas:

$$T_{m,j}(h)=h\{p_0(j)f_j+q_0(j)f_{j+1}\}+\sum_{k=1}^{m} h^{2k}\{\overline{p_k(j)}s_{2k-1,j}+\overline{q_k(j)}s_{2k-1,j+1}\}\quad (0\leq m\leq 3) \tag{16}$$

with $(\overline{p_k(j)}, \overline{q_k(j)})=(p_k(j), q_k(j))$ $(k=1, 2)$ and $(\overline{p_3(j)}, \overline{q_3(j)})=(p_3(j), q_3(j))+(p_1(j), q_1(j))/180$. As in the proof of Theorem 2, we have

**Theorem 3.** *Under the same assumption on k, m and f in Theorem 2,*

$$\int_{x_j}^{x_{j+1}} w(x)f(x)\,dx-T_{m,j}(h)=O(h^{2m+3+\min(0,\alpha)}) \text{ or } O(h^{2m+3}|\ln(h)|)\quad (0\leq m\leq 3)$$

*for* $w(x)=x^{\alpha}$ $(\alpha>-1)$ *or* $\ln(x)$.

Similarly we improve the trapezoidal rule for integrals of the form $\int_{x_j}^{x_{j+1}} w(x)f(x)\,dx$ with an oscillatory weight $w(x)=\cos(kx)$ or $\sin(kx)$ for a relatively large value of $k$. For $\cos(kx)$ or $\sin(kx)$, $c_m(=c_m(j))=\int_0^1 \theta^m\, w(x_j+h\theta)\,d\theta$ are determined by

$$\text{(17)}\quad \begin{aligned} &hkc_0(j)=\sin(kx_{j+1})-\sin(kx_j),\ h^2k^2c_1(j)=hk\sin(kx_{j+1})+\cos(kx_{j+1})-\cos(kx_j),\\ &h^2k^2c_m(j)=hk\sin(kx_{j+1})+m\cos(kx_{j+1})-m(m-1)c_{m-2}(j)\quad(m\geq 2)\end{aligned}$$

or

$$\text{(18)}\quad \begin{aligned} &hkc_0(j)=\cos(kx_j)-\cos(kx_{j+1}),\ h^2k^2c_1(j)=-hk\cos(kx_{j+1})-\sin(kx_{j+1})+\sin(kx_j)\\ &h^2k^2c_m(j)=-hk\cos(kx_{j+1})-m\sin(kx_{j+1})+m(m-1)c_{m-2}(j)\quad(m\geq 2).\end{aligned}$$

## 2. Numerical Examples

First, we consider an application of the above stated numerical formulas $S_{m,j}(h)$ and $M_{m,j}(h)$ by taking two functions $f(x)=\exp(5x)$ and $\sin(4\pi x)$. In Tables 1-4, are given the observed maximum absolute errors in the formulas on subintervals $[x_j, x_{j+1}]$ $(0\leq j\leq n-1)$ and the observed orders of convergence from the numerical results with $n=32, 64$. Figures in parentheses behind the observed orders of convergence are the theoretical ones predicted in Theorems where *a-b* means $a\times 10^{-b}$. For reference, the absolute errors in the composite formulas on the whole interval [0, 1] using $S_{m,j}(1/64)$ (or $M_{m,j}(1/64)$), $0\leq m\leq 3$ can be improved with a fixed umber of the evaluation points as 3.81-7 → 6.90-11 → 2.85-13 → 1.15-14 (or 7.50-3 → 1.33-6 → 1.76-9 → 1.92-12) where the orders of convergence in the composite rules using $S_{m,j}(h)$ (or $M_{m,j}(h)$) are approximately equal to the theoretical ones, $2m+5$ (or $2m+3$), respectively. Next, we consider an application of the product trapezoidal rule when $w(x)=1/\sqrt{x}$, $\ln(x)$ and 1 to the same functions $\exp(5x)$ and $\sin(4\pi x)$. We use $T_{3,j}(h/2)$ as the unknown exact values to bound the errors in $T_{m,j}(h)$ $(0\leq m\leq 2)$. In Table 4, note that the theoretical rates of convergence are different from the others since the maximum absolute errors occurred near at $x=0$. Finally we improve the product trapezoidal rule for evaluating two integrals [2]:

$$\text{(19)}\quad \int_{-1}^{1}(x-2)^{-1}(1-x)^{-1/4}(1+x)^{-3/4}\,dx\ (=-1.944905429166746\ldots)$$

$$\text{(20)}\quad \int_0^1 \exp(ux)\cos(kx)\,dx\ (=\exp(u)(u\cos k+k\sin k)-u)(u^2+k^2)^{-1})\quad(u=1, 5)$$

The integral (19) whose weight is singular at both end-points is subdivided at $x=0$ producing two integrals with a single end-point singularity. For (19), the absolute observed errors in the composite trapezoidal rule $\sum_{j=0}^{n-1} T_{m,j}(h)$ with $n=32$, i.e., 33 function evaluation points on $[-1, 1]$ were significantly improved as 1.82-5 → 1.43-7 → 4.40-9 → 1.28-10 for $0 \leq m \leq 3$. For (20) with 17 evaluation points, the observed absolute errors in evaluation of $\int_0^1 \exp(ux) \times \cos(kx)dx$ with $k=1$, 10, $10^2$, $10^3$, $10^4$ were given in Table 5. Our methods with a fixed number of evaluation points would be useful when finer meshes are not acceptable.

**Table 1.** Comparison of the maximum absolute errors in the numerical evaluation of $\int_{x_j}^{x_{j+1}} f(x)dx$ using improved Simpson's rules $S_{m,j}(h)$ $(0 \leq j \leq n-1)$

| $f(x)$ | nonperiodic $\exp(5x)$ | | | | periodic $\sin(4\pi x)$ | | | |
|---|---|---|---|---|---|---|---|---|
| $n \backslash m$ | 0 | 1 | 2 | 3 | 0 | 1 | 2 | 3 |
| 16 | 2.63-5 | 5.34-8 | 2.10-8 | 1.81-8 | 7.57-6 | 1.89-7 | 5.44-8 | 5.83-9 |
| 32 | 8.88-7 | 6.19-10 | 2.45-11 | 1.64-11 | 2.52-7 | 1.26-9 | 1.07-10 | 2.73-12 |
| 64 | 2.88-8 | 5.21-12 | 2.77-14 | 9.66-15 | 8.02-9 | 9.40-12 | 2.09-13 | 1.31-15 |
| orders | 4.9(5) | 6.9(7) | 9.8(9) | 10.7(11) | 5.0(5) | 7.1(7) | 9.0(9) | 11.0(11) |

**Table 2.** Comparison of the maximum absolute errors in the numerical evaluation of $\int_{x_j}^{x_{j+1}} f(x)dx$ using improved midpoint rulse $M_{m,j}(h)$ $(0 \leq j \leq n-1)$

| $f(x)$ | nonperiodic $\exp(5x)$ | | | | periodic $\sin(4\pi x)$ | | | |
|---|---|---|---|---|---|---|---|---|
| $n \backslash m$ | 0 | 1 | 2 | 3 | 0 | 1 | 2 | 3 |
| 16 | 3.23-2 | 9.02-5 | 1.98-6 | 8.45-8 | 1.47-3 | 9.97-5 | 3.90-6 | 4.56-7 |
| 32 | 4.37-3 | 3.09-6 | 1.65-8 | 8.61-11 | 1.97-4 | 9.10-7 | 3.03-8 | 8.68-10 |
| 64 | 5.67-4 | 1.01-7 | 1.34-10 | 1.56-13 | 2.50-5 | 2.83-8 | 2.36-10 | 1.68-12 |
| orders | 2.9(3) | 4.9(5) | 6.9(7) | 9.1(9) | 3.0(3) | 5.3(5) | 7.0(7) | 9.0(9) |

**Table 3.** Comparison of the maximum absolute errors in the numerical evaluation of $\int_{x_j}^{x_{j+1}} w(x)\sin(4\pi x)dx$ using improved product trapezoidal rules $T_{m,j}(h)$ $(0 \leq j \leq n-1)$

| $w(x)$ | | $x^{1-\sqrt{2}}$ | | | $\ln(x)$ | | | 1 | |
|---|---|---|---|---|---|---|---|---|---|
| $n \backslash m$ | 0 | 1 | 2 | 0 | 1 | 2 | 0 | 1 | 2 |
| 16 | 6.51-2 | 1.03-4 | 3.56-6 | 5.00-2 | 9.09-6 | 2.88-8 | 6.47-2 | 1-02-4 | 3.81-6 |
| 32 | 8.63-3 | 3.53-6 | 3.06-8 | 6.25-4 | 2.91-7 | 2.25-9 | 8.73-3 | 3.52-6 | 3.11-8 |
| 64 | 1.54-3 | 3.31-7 | 4.68-10 | 1.28-4 | 4.56-8 | 5.39-11 | 1.13-3 | 1.15-7 | 2.51-10 |
| orders | 2.5(2.5) | 3.4(4.5) | 6.0(6.5) | 2.3(2.7) | 2.7(4.7) | 5.4(6.7) | 2.9(3) | 4.9(5) | 7.0(7) |

**Table 4.** Comparison of the maximum absolute errors in the numerical evaluation of $\int_{x_j}^{x_{j+1}} w(x)\exp(5x)\,dx$ using improved product trapezoidal rules $T_{m,j}(h)$ $(0 \leq j \leq n-1)$

| $w(x)$ | | $x^{1-\sqrt{2}}$ | | | $\ln(x)$ | | | 1 | |
|---|---|---|---|---|---|---|---|---|---|
| $n \backslash m$ | 0 | 1 | 2 | 0 | 1 | 2 | 0 | 1 | 2 |
| 16 | 9.55-3 | 7.99-5 | 1.32-7 | 7.15-3 | 7.08-5 | 1.01-8 | 2.92-3 | 3.68-5 | 7.23-6 |
| 32 | 1.97-3 | 2.53-6 | 1.69-9 | 8.98-4 | 2.24-6 | 8.00-10 | 3-92-4 | 1.06-6 | 5.68-8 |
| 64 | 5.52-4 | 1.29-7 | 2.92-11 | 1.60-4 | 7.11-8 | 9.54-12 | 4.99-5 | 3.25-8 | 4.44-10 |
| orders | 1.8(2.5) | 4.3(4.5) | 5.9(6.5) | 2.5(2.7) | 4.7(4.7) | 6.5(6.7) | 3.0(3) | 5.0(5) | 7.0(7) |

**Table 5.** Comparison of the maximum absolute errors in the numerical evaluation of $\int_0^1 \exp(ux)\cos(kx)\,dx$ using composite improved product trapezoidal rules $\sum_{j=0}^{n-1} T_{m,j}(h)$

| $u$ | | 1 | | | | 5 | | |
|---|---|---|---|---|---|---|---|---|
| $k \backslash m$ | 0 | 1 | 2 | 3 | 0 | 1 | 2 | 3 |
| 1 | 3.84-4 | 2.73-8 | 3.50-11 | 2.03-14 | 1.55-1 | 2.49-4 | 8.77-6 | 3.45-8 |
| 10 | 2.33-4 | 9.01-9 | 2.41-11 | 1.40-14 | 1.18-1 | 1.60-4 | 6.63-6 | 1.13-7 |
| $10^2$ | 1.88-3 | 6.45-8 | 1.63-10 | 9.00-14 | 2.70-1 | 2.94-4 | 1.47-5 | 1.07-7 |
| $10^3$ | 9.30-8 | 3.10-11 | 8.61-15 | 4.88-18 | 1.61-4 | 4-36-7 | 9.05-9 | 4.19-10 |
| $10^4$ | 3.59-8 | 4.6-15 | 3.04-15 | 1.42-18 | 7.12-6 | 3.75-10 | 3.78-10 | 4.06-12 |

## References


[1] J. Ahlberg, E. Nilson and J. Walsh, Theory of Splines and Their Applications, Academic Press, New York, 1967.

[2] G. Evans, Practical Numerical Integration, John Wiley & Sons, New York, 1993.

[3] M. Sakai and R. Usmani, On consistency relations for cubic splines-on-splines and their asymptotic error estimates, J. Approx. Theory, **55**(1985), 195–200.

[4] M. Sakai and R. Usmani, On spline-on-spline numerical integration formula, J. Approx. Theory, **59** (1989), 350–355.

[5] M. Sakai and R. Usmani, Numerical integration formulas based on iterated cubic splines, Computing, **52**(1994), 309–314.

[6] M. Shelly and G. Baker, On order-preserving approximation to successive derivatives of periodic functions by iterated splines, SIAM J. Numer. Anal., **25**(1988), 1442–1452.